



Yasuda-Shedlovsky Result

Sample name: **CS000204**
Assay name: **pH-metric psKa**
Assay ID: **11I-13017**
Filename: **E:\T3 DATA\1109\11I-13017_CS000204_pH-metric psKa.t3r**

Experiment start time: **13/09/2011 20:22:31**
Analyst:
Instrument ID: **T311042**

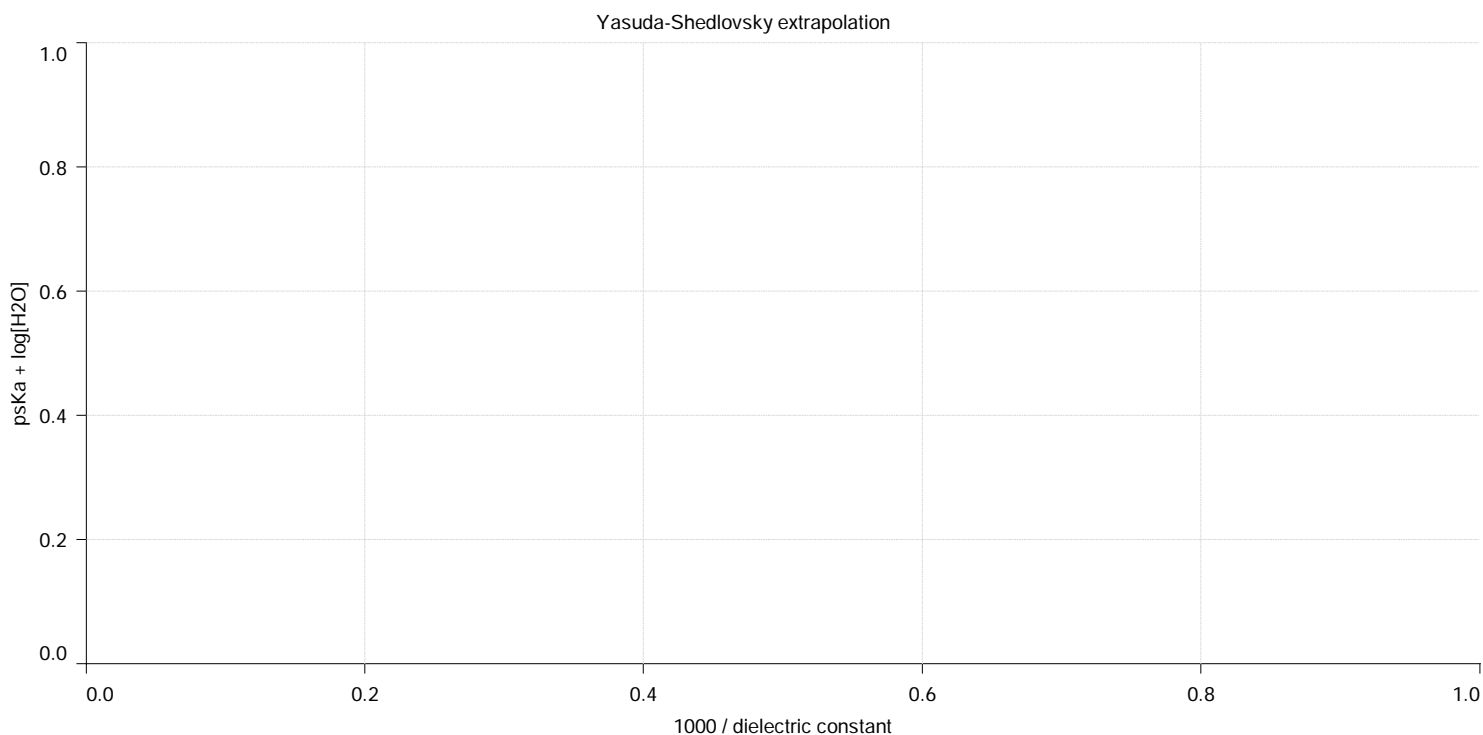
Yasuda-Shedlovsky result

Extrapolation type pKa 0% SD Intercept Slope R² Ionic strength Temperature

Component assay results

| Titration | DMSO weight% | Direction | Result type | Dielectric constant | [H ₂ O] | Ionic strength | Temperature |
|---------------------------|--------------|-----------|-------------|---------------------|--------------------|----------------|-------------|
| 11I-13017 Points 62 to 99 | 23.08 % | Up | pH-metric | 76.5 | 43.4 M | 0.189 M | 27.5°C |
| 11I-13017 Points 30 to 61 | 30.15 % | Up | pH-metric | 76.3 | 39.7 M | 0.183 M | 27.0°C |
| 11I-13017 Points 3 to 29 | 38.56 % | Up | pH-metric | 75.9 | 35.2 M | 0.171 M | 26.1°C |

Graphs



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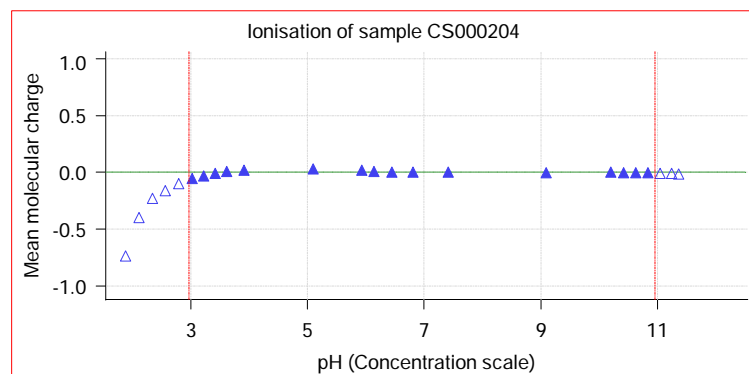
Filename: **E:\T3 DATA\1109\11I-13017_CS000204_pH-metric psKa.t3r**

pH-metric psKa Titration 1 of 3 11I-13017 Points 3 to 29

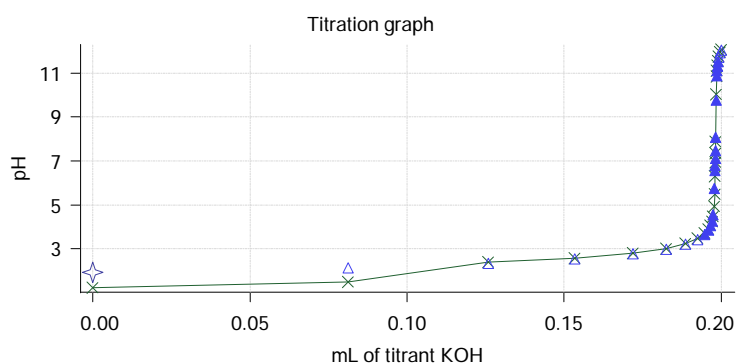
Sample

 CS000204 concentration factor 0.923

Sample graphs



Other graphs



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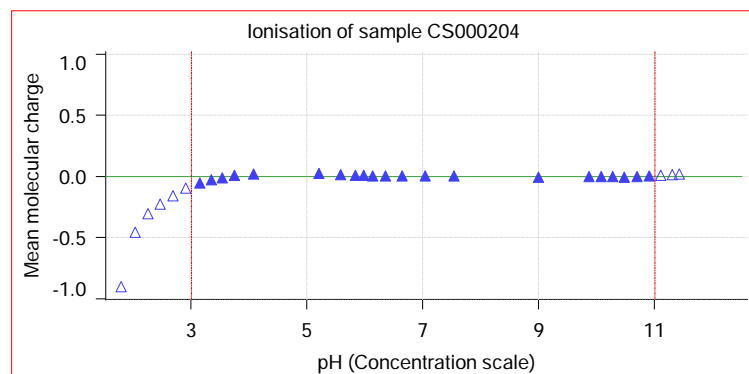
Experiment start time: **13/09/2011 20:22:31**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11I-13017 Points 30 to 61

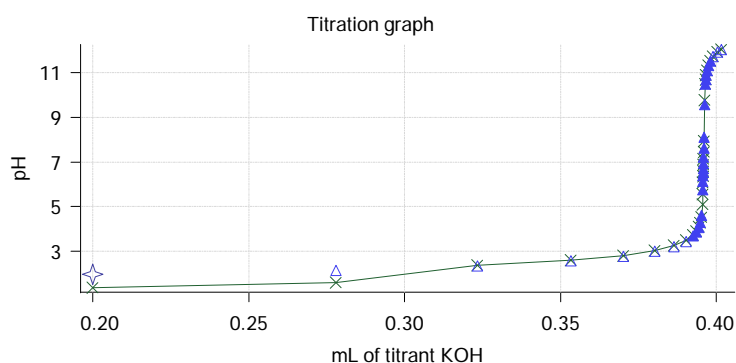
Sample

 CS000204 concentration factor 0.948

Sample graphs



Other graphs




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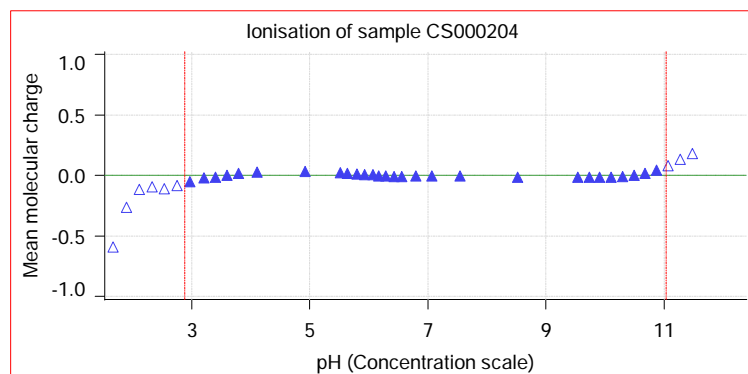
Experiment start time: **13/09/2011 20:22:31**
 Analyst:
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pH-metric psKa Titration 3 of 3 11I-13017 Points 62 to 99

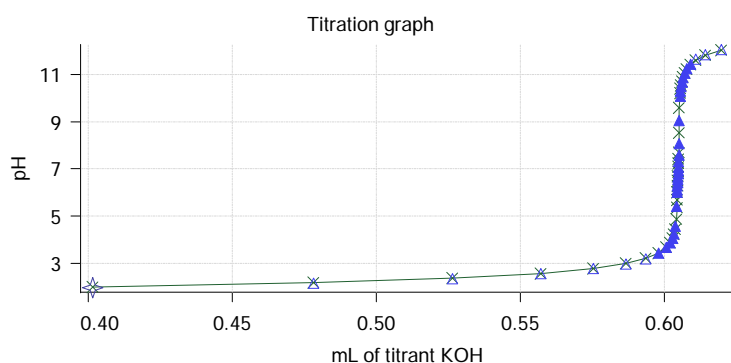
Sample

 CS000204 concentration factor 1.114

Sample graphs



Other graphs



Assay Model

| Settings | Value | Date/Time changed | Imported from |
|-----------------------------------|--------------|-------------------|---------------|
| Sample name | CS000204 | | |
| Sample by | Weight | | |
| Sample weight | 0.000960 g | | |
| Formula weight | 349.34 g/mol | | |
| Solubility | Unknown | | |
| Molecular weight | 349.34 | | |
| Individual pKa ionic environments | No | | |
| Number of pKas | 0 | | |
| logP (neutral X) | -10.00 | | |